Welcome to STN International! Enter x:x

LOGINID: SSPTANXR1625

specific topic.

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

```
Welcome to STN International
NEWS
                 Web Page for STN Seminar Schedule - N. America
         MAR 15 WPIDS/WPIX enhanced with new FRAGHITSTR display format
NEWS 2
NEWS 3
         MAR 16 CASREACT coverage extended
NEWS 4 MAR 20 MARPAT now updated daily
NEWS 5 MAR 22 LWPI reloaded
NEWS 6 MAR 30 RDISCLOSURE reloaded with enhancements
NEWS 7 APR 02 JICST-EPLUS removed from database clusters and STN
NEWS 8 APR 30 GENBANK reloaded and enhanced with Genome Project ID field
         APR 30 CHEMCATS enhanced with 1.2 million new records
NEWS 9
         APR 30 CA/CAplus enhanced with 1870-1889 U.S. patent records
NEWS 10
NEWS 11
         APR 30
                 INPADOC replaced by INPADOCDB on STN
NEWS 12
         MAY 01
                 New CAS web site launched
NEWS 13
         MAY 08
                 CA/CAplus Indian patent publication number format defined
NEWS 14
         MAY 14
                 RDISCLOSURE on STN Easy enhanced with new search and display
NEWS 15
         MAY 21
                 BIOSIS reloaded and enhanced with archival data
NEWS 16
         MAY 21
                 TOXCENTER enhanced with BIOSIS reload
NEWS 17
         MAY 21
                 CA/CAplus enhanced with additional kind codes for German
                 patents
NEWS 18
         MAY 22
                 CA/CAplus enhanced with IPC reclassification in Japanese
                 patents
NEWS 19
         JUN 27
                 CA/CAplus enhanced with pre-1967 CAS Registry Numbers
NEWS 20 JUN 29
                 STN Viewer now available
NEWS 21
         JUN 29
                 STN Express, Version 8.2, now available
NEWS 22 JUL 02 LEMBASE coverage updated
NEWS 23 JUL 02 LMEDLINE coverage updated
NEWS 24 JUL 02 SCISEARCH enhanced with complete author names
NEWS 25
         JUL 02 CHEMCATS accession numbers revised
NEWS 26
         JUL 02
                 CA/CAplus enhanced with utility model patents from China
NEWS 27
         JUL 16 CAplus enhanced with French and German abstracts
NEWS 28
         JUL 18 CA/CAplus patent coverage enhanced
NEWS EXPRESS 29 JUNE 2007: CURRENT WINDOWS VERSION IS V8.2,
              CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0jc(JP),
              AND CURRENT DISCOVER FILE IS DATED 05 JULY 2007.
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              STN Operating Hours Plus Help Desk Availability
NEWS LOGIN
              Welcome Banner and News Items
              For general information regarding STN implementation of IPC 8
NEWS IPC8
Enter NEWS followed by the item number or name to see news on that
```

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=> file reg

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION

0.21

0.21

FULL ESTIMATED COST

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http://www.cas.org/support/stngen/stndoc/properties.html

=>

Uploading C:\Program Files\Stnexp\Queries\10567314.str

chain nodes: 10 12 13

ring nodes :

1 2 3 4 5 6 7 8 9

chain bonds : 4-12 6-13 7-10

ring bonds :

1-2 1-6 1-7 2-3 2-9 3-4 4-5 5-6 7-8 8-9

exact/norm bonds :

1-2 1-6 1-7 2-3 3-4 4-5 4-12 5-6 6-13 7-10

exact bonds:
2-9 7-8 8-9
isolated ring systems:
containing 1:

Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 12:Atom 13:Atom

L1 STRUCTURE UPLOADED

=> d l1 L1 HAS NO ANSWERS L1 STR

Structure attributes must be viewed using STN Express query preparation.

=> s 11

SAMPLE SEARCH INITIATED 06:31:57 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 2465 TO ITERATE

81.1% PROCESSED 2000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

O ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

46322 TO 52278

PROJECTED ANSWERS: 0 TO (

L2 0 SEA SSS SAM L1

=> s l1 full

FULL SEARCH INITIATED 06:32:01 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 50347 TO ITERATE

100.0% PROCESSED 50347 ITERATIONS SEARCH TIME: 00.00.01

2 ANSWERS

L3

2 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE TOTAL ENTRY SESSION 172.10 172.31

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FILE COVERS 1907 - 26 Jul 2007 VOL 147 ISS 5 FILE LAST UPDATED: 25 Jul 2007 (20070725/ED)

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http://www.cas.org/infopolicy.html

=> s 13 full

L4 1 L3

=> d ibib abs hitstr tot

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:177892 CAPLUS

DOCUMENT NUMBER:

142:280058

TITLE:

Preparation of bicyclic terahydropyridine compounds as

mitotic kinesin inhibitors for treating cancer

INVENTOR(S):

Coleman, Paul J.

PATENT ASSIGNEE(S):

Merck & Co., Inc., USA PCT Int. Appl., 114 pp.

SOURCE:

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

': 1

PATENT INFORMATION:

PATENT NO.				KIND		DATE		APPLICATION NO.					DATE				
WO 2005018638				A1 20050303			WO 2004-US25856					20040809					
	W:	ΑE,	AG,	AL,	AM,	AT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BW,	BY,	ΒZ,	CA,	CH,
							DE,										
							ID,										
							LV,										
		NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RŲ,	SC,	SD,	SE,	SG,	SK,	SL,	SY,
		ТJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW
	RW:	BW,	GH,	GM,	ΚE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	.ZW,	AM,
		ΑZ,	BY,	KG,	ΚZ,	MD,	RU,	ТJ,	TM,	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,
		EE,	ES,	FI,	FR,	GB,	GR,	HU,	IE,	IT,	LU,	MC,	NL,	PL,	·PT,	RO,	SE,
							CF,										
			TD,														

AU 2004266612	· A1	20050303	AU 2004-266612		20040809		
· CA 2533435	A1	20050303	CA 2004-2533435		20040809		
EP 1656140	Al	20060517	EP 2004-780658	•	20040809		
R: AT, BE,	CH, DE,	DK, ES, FR,	GB, GR, IT, LI, LU,	NL,	SE, MC, PT,		
IE, SI,	LT, LV,	FI, RO, CY,	TR, BG, CZ, EE, HU,	PL,	SK		
CN 1835749 ,	A	20060920	CN 2004-80023220		20040809		
JP 2007502279	. T	20070208	JP 2006-523301		20040809		
US 2006223844	A1	20061005	US 2006-567314		20060207		
PRIORITY APPLN. INFO). :		US 2003-494670P	· P	20030813		
			WO 2004-US25856	W	20040809		
OTHER SOURCE(S):	CAS	REACT 142:280	0058; MARPAT 142:280	058			

Ι

III

GI

IV

AB The present invention relates to bicyclic terahydropyridine compds. I [X =SO, SO2, CO, (un) substituted (CH2) v; Y = O, S, CO, etc.; or X and Y are combined to form (un) substituted CH:CH; Z = CO, CS, SO, SO2, (un) substituted CH2; or Y and Z are combined to form (un) substituted N:CH; R1, R4 = aryl, aralkyl, cycloalkyl, heterocyclyl; R2, R31, R32, R5-R7 = H, alkyl, aryl, etc.; v = 1-3] that are useful for treating cellular proliferative diseases, for treating disorders associated with KSP kinesin activity, and for inhibiting KSP kinesin. E.g., a 2-step synthesis of (-)-(5S,8aR)-II and (+)-(5S,8aR)-III (separated), starting from bicyclic piperidone IV, which showed (both) an IC50 of ≤ 50 µM in kinesin ATPase in vitro assay, was given. The invention is also related to compns. which comprise these compds. I, and methods of using them to treat cancer in mammals.

IT 847049-58-5P 847049-60-9P

II

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of bicyclic terahydropyridine compds. as mitotic kinesin inhibitors for treating or preventing cancer)

RN 847049-58-5 CAPLUS

3(2H)-Indolizinone, 7-(2,5-difluorophenyl)-1,5,8,8a-tetrahydro-5-phenyl-, CN (5S,8aR) - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 847049-60-9 CAPLUS

CN 3(2H)-Indolizinone, 7-(2,5-difluorophenyl)-1,5,6,8a-tetrahydro-5-phenyl-, (5S,8aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

REFERENCE COUNT:

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d his

(FILE 'HOME' ENTERED AT 06:31:28 ON 26 JUL 2007)

3

FILE 'REGISTRY' ENTERED AT 06:31:37 ON 26 JUL 2007

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 2 S L1 FULL

FILE 'CAPLUS' ENTERED AT 06:32:07 ON 26 JUL 2007

L4 1 S L3 FULL

=> log y COST IN U.S. DOLLARS SINCE FILE ENTRY SESSION FULL ESTIMATED COST 5.74 178.05 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION CA SUBSCRIBER PRICE -0.78-0.78

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     1
                Web Page for STN Seminar Schedule - N. America
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        MAR 15 WPIDS/WPIX enhanced with new FRAGHITSTR display format
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     7 APR 02 JICST-EPLUS removed from database clusters and STN
NEWS 8 APR 30 GENBANK reloaded and enhanced with Genome Project ID field
NEWS 9 APR 30
                CHEMCATS enhanced with 1.2 million new records
NEWS 10 APR 30 CA/CAplus enhanced with 1870-1889 U.S. patent records
NEWS 11 APR 30
                INPADOC replaced by INPADOCDB on STN
NEWS 12
        MAY 01
                New CAS web site launched
NEWS 13
        MAY 08
                CA/CAplus Indian patent publication number format defined
NEWS 14
        MAY 14
                RDISCLOSURE on STN Easy enhanced with new search and display
NEWS 15
        MAY 21
                BIOSIS reloaded and enhanced with archival data
NEWS 16
        MAY 21
                 TOXCENTER enhanced with BIOSIS reload
NEWS 17
        MAY 21
                CA/CAplus enhanced with additional kind codes for German
                 patents
NEWS 18
        MAY 22
                CA/CAplus enhanced with IPC reclassification in Japanese
                patents
NEWS 19
         JUN 27
                CA/CAplus enhanced with pre-1967 CAS Registry Numbers
NEWS 20 JUN 29
                STN Viewer now available
NEWS 21. JUN 29
                STN Express, Version 8.2, now available
NEWS 22 JUL 02
                LEMBASE coverage updated
NEWS 23 JUL 02 LMEDLINE coverage updated
NEWS 24 JUL 02 SCISEARCH enhanced with complete author names
         JUL 02 CHEMCATS accession numbers revised
NEWS 25
         JUL 02 CA/CAplus enhanced with utility model patents from China
NEWS 26
NEWS 27
         JUL 16 CAplus enhanced with French and German abstracts
NEWS 28 JUL 18 CA/CAplus patent coverage enhanced
NEWS EXPRESS 29 JUNE 2007: CURRENT WINDOWS VERSION IS V8.2,
             CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
             AND CURRENT DISCOVER FILE IS DATED 05 JULY 2007.
NEWS HOURS
              STN Operating Hours Plus Help Desk Availability
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              Welcome Banner and News Items
NEWS IPC8
              For general information regarding STN implementation of IPC 8
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=> file reg

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SINCE FILE TOTAL ENTRY SESSION 0.21 0.21

FULL ESTIMATED COST

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TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

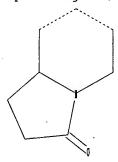
Please note that search-term pricing does apply when conducting SmartSELECT searches.

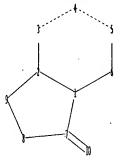
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http://www.cas.org/support/stngen/stndoc/properties.html

=>

Uploading C:\Program Files\Stnexp\Queries\10567314a.str





chain nodes :

10

ring nodes :

1 2 3 4 5 6 7 8 9

chain bonds :

7-10

ring bonds :

1-2 1-6 1-7 2-3 2-9 3-4 4-5 5-6 7-8 8-9

exact/norm bonds :

1-2 1-6 1-7 2-3 3-4 4-5 5-6 7-10

exact bonds :

2-9 7-8 8-9

isolated ring systems :

containing 1:

Match level:

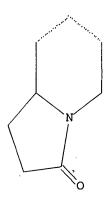
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS

STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1



Structure attributes must be viewed using STN Express query preparation.

44 ANSWERS

962 ANSWERS

=> s 11

SAMPLE SEARCH INITIATED 06:36:59 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 2465 TO ITERATE

81.1% PROCESSED 2000 ITERATIONS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**.

PROJECTED ITERATIONS: 46322 TO 52278

PROJECTED ANSWERS: 643 TO

44 SEA SSS SAM L1

=> s 11 full

FULL SEARCH INITIATED 06:37:07 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 50347 TO ITERATE

100.0% PROCESSED 50347 ITERATIONS

SEARCH TIME: 00.00.01

962 SEA SSS FUL L1

=> d 1-2

L3 ANSWER 1 OF 962 REGISTRY COPYRIGHT 2007 ACS on STN

942603-62-5 REGISTRY RN

Entered STN: 18 Jul 2007

CN 8a(1H)-Indolizinecarboxylic acid, 2,3,5,8-tetrahydro-3-oxo-, ethyl ester

(CA INDEX NAME)

MF C11 H15 N O3

SR CA

LC STN Files: CAPLUS

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 2 OF 962 REGISTRY COPYRIGHT 2007 ACS on STN

RN 937818-67-2 REGISTRY

ED Entered STN: 19 Jun 2007

CN 3(2H)-Indolizinone, 5-(4-fluorophenyl)hexahydro-2-[[3-methoxy-4-(4-methyl-1H-imidazol-1-yl)phenyl]methylene]-, (2E,5R,8aS)-rel- (CA INDEX NAME)

FS STEREOSEARCH

MF C26 H26 F N3 O2

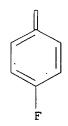
SR CA

LC STN Files: CA, CAPLUS, USPATFULL

Relative stereochemistry.

Double bond geometry as shown.

PAGE 1-A



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file caplus
COST IN U.S. DOLLARS

SINCE FILE

TOTAL

FULL ESTIMATED COST

ENTRY

SESSION

176.45

176.66

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=> s 13 full

L4 357 L3

=> s 14 and py<2003 22882984 PY<2003

L5 298 L4 AND PY<2003

=> d ibib abs hitstr 100-110

L5 ANSWER 100 OF 298 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

1995:786681 CAPLUS

DOCUMENT NUMBER:

123:228598

TITLE:

Enantioselective total synthesis of (-)-indolizidines 209B and 209D via a highly efficient aza-[2,3]-Wittig.

rearrangement of vinylaziridines

AUTHOR(S):

Aehman, Jens; Somfai, Peter

CORPORATE SOURCE:

Chemical Center Lund Institute Technology, University

Lund, Lund, S-221 00, Swed.

SOURCE:

Tetrahedron (1995), 51(35), 9747-56

CODEN: TETRAB; ISSN: 0040-4020

PUBLISHER:

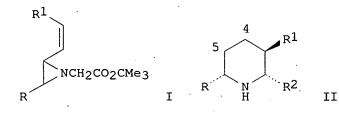
DOCUMENT TYPE:

LANGUAGE:

OTHER SOURCE(S):

Elsevier Journal English

CASREACT 123:228598



AΒ A novel protocol for the enantioselective synthesis of (-)-indolizidines 209B and 209D is described in which the key step is the highly efficient aza-[2,3]-Wittig rearrangement of vinylaziridines I (R = hexyl, R1 = H, R = pentyl, R1 = Me) into tetrahydropyridines II (R2 = CO2CMe3, 4,5-unsatd.). Functional group manipulation and chain elongation then gave esters II [R2 = (CH2)2CO2Et, 4,5-saturated] which were converted to the target alkaloids via the resp. indolizidine lactams.

161404-23-5P 168421-40-7P

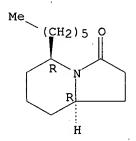
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(enantioselective total synthesis of indolizidines 209B and 209D via aza-[2,3]-Wittig rearrangement of vinylaziridines)

RN 161404-23-5 CAPLUS

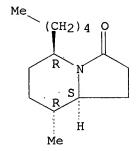
3(2H)-Indolizinone, 5-hexylhexahydro-, (5R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN168421-40-7 CAPLUS

3(2H)-Indolizinone, hexahydro-8-methyl-5-pentyl-, [5R-CN $(5\alpha, 8\beta, 8a\beta)$] - (9CI) (CA INDEX NAME)



ANSWER 101 OF 298 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

1995:761247 CAPLUS

DOCUMENT NUMBER:

123:228586

TITLE:

Asymmetric synthesis of indolizidines 167B and 223AB

AUTHOR(S): CORPORATE SOURCE: Takahata, Hiroki; Bandoh, Hiroshi; Momose, Takefumi Faculty of Pharmaceutical Sciences, Toyama Medical &

Pharmaceutical University, Toyama, 930-01, Japan

SOURCE:

Heterocycles (1995), 41(8), 1797-804

CODEN: HTCYAM; ISSN: 0385-5414

PUBLISHER:

Japan Institute of Heterocyclic Chemistry

DOCUMENT TYPE:

Journal

LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 123:228586

GΙ

AB The total synthesis of (+)-indolizidine 167B (I) and the formal synthesis of (-)-indolizidine 223AB starting with L- and D-norvaline-derived cis-2-hydroxymethyl-6-propylpiperidines, resp., were achieved.

IT 168610-24-0P

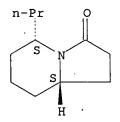
> RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(asym. synthesis of indolizidines 167B and 223AB)

RN168610-24-0 CAPLUS

CN 3(2H)-Indolizinone, hexahydro-5-propyl-, (5S-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



L5 ANSWER 102 OF 298 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1995:741428 CAPLUS

DOCUMENT NUMBER: 123:227609

TITLE: Photocatalyzed multiple additions of amines to

 α , β -unsaturated esters and nitriles.

[Erratum to document cited in CA120:298026]

AUTHOR(S): Das, Suresh; Kumar, J. S. Dileep; Thomas, K. George;

Shivaramayya, K.; George, M. V.

CORPORATE SOURCE: Reg. Res. Lab., CSIR, Trivandrum, 695 019, India

SOURCE: Journal of Organic Chemistry (1995), 60(15),

4958

CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal LANGUAGE: English

AB The errors were not reflected in the abstract or the index entries.

·IT 155068-03-4P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of (Erratum))

RN 155068-03-4 CAPLUS

CN 3(2H)-Indolizinone, hexahydro-2-methyl- (9CI) (CA INDEX NAME)

L5 ANSWER 103 OF 298 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1995:722743 CAPLUS

DOCUMENT NUMBER: 123:339545

TITLE: Anthraquinone-photocatalyzed addition of amines to

 α,β -unsaturated esters: a novel route to

indolizidone, pyrrolizidone and related ring systems AUTHOR(S): Das, Suresh; Kumar, J. S. Dileep; Shivaramayya, K.;

George, M. V.

CORPORATE SOURCE: Photochem. Res. Unit, Reg. Res. Lab. (CSIR),

Trivandrum, 695 019, India

SOURCE: Journal of the Chemical Society, Perkin Transactions

1: Organic and Bio-Organic Chemistry (1995),

(14), 1797-9

CODEN: JCPRB4; ISSN: 0300-922X

PUBLISHER:

Royal Society of Chemistry

DOCUMENT TYPE:

Journal

LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 123:339545

AB An indolizidone, a pyrrolizidone, a mixture of heliotridone and pseudoheliotridone and a lactam have been synthesized in a one-step anthraquinone-photocatalyzed reaction of piperidine, pyrrolidine, and morpholine with α,β -unsatd. esters.

IT 2740-00-3P

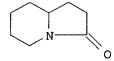
RL: SPN (Synthetic preparation); PREP (Preparation)

(anthraquinone-photocatalyzed addition of amines to α,β -unsatd.

esters)

RN 2740-00-3 CAPLUS

CN 3(2H)-Indolizinone, hexahydro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



L5 ANSWER 104 OF 298 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1995:610345 CAPLUS

DOCUMENT NUMBER: 123:228886

TITLE: Constrained C-terminal hexapeptide neurotensin analogs

containing a 3-oxoindolizidine skeleton

AUTHOR(S): Garcia-Loper, M. Teresa; Akorta, Ibon; Dominguez, M.

Jose; Gonzalez-Muniz, Rosario; Herranz, Rosario;

Johansen, Nils L.; Madsen, Kjeld; Thoegersen, Henning;

Suzdak, Peter

CORPORATE SOURCE:

Instituto Quimica Medica, Madrid, E-28006, Spain

SOURCE:

Letters in Peptide Science (1995), 1(6),

269-76

CODEN: LPSCEM; ISSN: 0929-5666

PUBLISHER: DOCUMENT TYPE:

ESCOM

LANGUAGE:

Journal English

CT

H-Arg-Arg-NH

IT

I

AΒ In order to enforce different spatial orientations in the C-terminal hexapeptide of neurotensin (NT8-13) and to gain information about the importance of the 10-11 peptide bond for binding to NT receptors, the Pro10-Tyr11 fragment has been replaced with (2R,8S,8aR)-, (2S,8S,8aS)-, and (2R,8R,8aS)-8-amino-2-benzyl-3-oxoindolizidine-2-carboxylic acid. Mol. dynamics calcns. and energy minimization studies have shown that, in contrast to the Pro-Tyr moiety, none of these indolizines display a tendency to adopt type I and III β -turns, but those having (8S,8aR) or (8R,8aS) stereochem. essentially adopt extended conformations and the (8S, 8aS) stereoisomer prefers a nonstandard folding. The four diastereomeric NT8-13 analogs I incorporating (8S,8aR) or (8R,8aS) indolizidines displayed binding affinities for the brain NT receptor similar to that of [Ala11]-NT8-13 and only five- to ninefold lower than that of the corresponding analog, [Phell]-NT8-13. Although this light decrease could be attributed to differences in conformation behavior between these constrained NT8-13 analogs and [Phe11]NT8-13 or NT8-13, it is not clear whether the β -turn around Pro10-AA11 (AA = Phe, Tyr) is conserved upon receptor binding. An excessive restriction in the motions of the aromatic side chain, imposed by the highly steric constraint of the indolizidine moiety, emerges as an alternative explanation. The findings reported here demonstrate the possibility of replacing the Pro10-Tyr11 dipeptide in NT8-13 with a nonpeptide residue without affecting considerably the affinity for brain NT receptors.

158668-67-8P 158706-01-5P 158706-02-6P

168608-95-5P 168608-96-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation of constrained C-terminal hexapeptide neurotensin analogs containing stereoisomeric oxoindolizidine skeletons)

RN 158668-67-8 CAPLUS

CN L-Leucine, N-[N-[[8-[(N2-L-arginyl-L-arginyl)amino]octahydro-3-oxo-2-(phenylmethyl)-2-indolizinyl]carbonyl]-L-isoleucyl]-, [2S-(2 α ,8 β ,8a β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 158706-01-5 CAPLUS

CN L-Leucine, N-[N-[[8-[(N2-L-arginyl-L-arginyl)amino]octahydro-3-oxo-2-(phenylmethyl)-2-indolizinyl]carbonyl]-L-isoleucyl]-, [2R-(2\alpha,8\alpha\alpha)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 158706-02-6 CAPLUS

CN L-Leucine, N-[N-[[8-[(N2-L-arginyl-L-arginyl)amino]octahydro-3-oxo-2-(phenylmethyl)-2-indolizinyl]carbonyl]-L-isoleucyl]-, [2R-(2α,8α,8aβ)]- (9CI) (CA INDEX NAME)

$$H_{2N}$$
 H_{2N}
 H

RN 168608-95-5 CAPLUS

CN L-Leucine, N-[N-[[8-[(N2-L-arginyl-L-arginyl)amino]octahydro-3-oxo-2-(phenylmethyl)-2-indolizinyl]carbonyl]-L-isoleucyl]-, [2R-(2 α ,8 β ,8a β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 168608-96-6 CAPLUS

CN L-Leucine, N-[N-[[8-[(N2-L-arginyl-L-arginyl)amino]octahydro-3-oxo-2-(phenylmethyl)-2-indolizinyl]carbonyl]-L-isoleucyl]-, [2S-(2\alpha, 8\alpha, 8\alpha)]- (9CI) (CA INDEX NAME)

IT 168336-94-5 168608-97-7 168608-98-8

168608-99-9 168609-00-5

RL: PRP (Properties)

(preparation of constrained C-terminal hexapeptide neurotensin analogs containing stereoisomeric oxoindolizidine skeletons)

RN 168336-94-5 CAPLUS

CN 2-Indolizinecarboxamide, 8-(acetylamino)octahydro-N-methyl-3-oxo-2-(phenylmethyl)-, $[2S-(2\alpha,8\beta,8a\beta)]-(9CI)$ (CA INDEX NAME)

Absolute stereochemistry.

RN 168608-97-7 CAPLUS

CN 2-Indolizinecarboxamide, 8-(acetylamino)octahydro-N-methyl-3-oxo-2-(phenylmethyl)-, [2R- $(2\alpha, 8\alpha, 8a\alpha)$]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 168608-98-8 CAPLUS

CN 2-Indolizinecarboxamide, 8-(acetylamino)octahydro-N-methyl-3-oxo-2-(phenylmethyl)-, $[2R-(2\alpha,8\alpha,8a\beta)]-(9CI)$ (CA INDEX NAME)

RN 168608-99-9 CAPLUS

CN 2-Indolizinecarboxamide, 8-(acetylamino)octahydro-N-methyl-3-oxo-2-(phenylmethyl)-, $[2R-(2\alpha,8\beta,8a\beta)]-(9CI)$ (CA INDEX NAME)

Absolute stereochemistry.

RN 168609-00-5 CAPLUS

CN 2-Indolizinecarboxamide, 8-(acetylamino)octahydro-N-methyl-3-oxo-2- (phenylmethyl)-, [2S-(2α , 8α , $8a\alpha$)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 168336-93-4 168608-91-1 168608-92-2

168608-93-3 168608-94-4

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of constrained C-terminal hexapeptide neurotensin analogs containing stereoisomeric oxoindolizidine skeletons)

RN 168336-93-4 CAPLUS

CN 2-Indolizinecarboxylic acid, 8-aminooctahydro-3-oxo-2-(phenylmethyl)-, [2R- $(2\alpha,8\beta,8a\beta)$]- (9CI) (CA INDEX NAME)

RN 168608-91-1 CAPLUS

CN 2-Indolizinecarboxylic acid, 8-aminooctahydro-3-oxo-2-(phenylmethyl)-, $[2S-(2\alpha,8\alpha,8a\alpha)]-(9CI)$ (CA INDEX NAME)

Absolute stereochemistry.

RN 168608-92-2 CAPLUS

CN 2-Indolizinecarboxylic acid, 8-aminooctahydro-3-oxo-2-(phenylmethyl)-, [2S-(2\alpha,8\alpha,8\alpha)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 168608-93-3 CAPLUS

CN 2-Indolizinecarboxylic acid, 8-aminooctahydro-3-oxo-2-(phenylmethyl)-, [2S- $(2\alpha, 8\beta, 8a\beta)$]- (9CI) (CA INDEX NAME)

RN 168608-94-4 CAPLUS

CN 2-Indolizinecarboxylic acid, 8-aminooctahydro-3-oxo-2-(phenylmethyl)-, $[2R-(2\alpha,8\alpha,8a\alpha)]-(9CI)$ (CA INDEX NAME)

Absolute stereochemistry.

L5 ANSWER 105 OF 298 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

1995:593950 CAPLUS

DOCUMENT NUMBER:

123:56338

TITLE:

Stereoselective synthesis of (+)-swainsonine and

(-)-8,8a-di-epi-swainsonine

AUTHOR(S):

Oishi, Tohru; Iwakuma, Toshihiro; Hirama, Masahiro;

Ito, Sho

CORPORATE SOURCE:

Dep. Chemistry, Tohoku Univ., Sendai, 980-77, Japan

SOURCE:

Synlett (1995), (5), 404-6

PUBLISHER:

CODEN: SYNLES; ISSN: 0936-5214 Thieme

DOCUMENT TYPE:

Journal

LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 123:56338

GI

RN

AB (+)-Swainsonine (I) and (-)-8,8a-di-epi-swainsonine (II) were stereoselectively synthesized from L-glutamic acid via a highly diastereoselective intramol. conjugate addition of amide III and carbamate IV, resp. Another key step is a stereoselective osmium-catalyzed dihydroxylation of indolizidine double bond.

IT 164739-28-0P 164739-29-1P 164739-30-4P

III

Ι

164739-32-6P 164907-55-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

IV

(stereoselective synthesis of (+)-swainsonine and (-)-epi-swainsonine) 164739-28-0 CAPLUS

CN 3(2H)-Indolizinone, 8-[[(1,1-dimethylethyl)dimethylsilyl]oxy]hexahydro-2-(trimethylsilyl)- (9CI) (CA INDEX NAME)

RN 164739-29-1 CAPLUS

CN 3(2H)-Indolizinone, 8-[[(1,1-dimethylethyl)dimethylsilyl]oxy]hexahydro-, (8S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 164739-30-4 CAPLUS

CN 3(2H)-Indolizinone, 8-[[(1,1-dimethylethyl)dimethylsilyl]oxy]hexahydro-2-(phenylseleno)- (9CI) (CA INDEX NAME)

RN 164739-32-6 CAPLUS

CN 3(2H)-Indolizinone, 8-[[(1,1-dimethylethyl)dimethylsilyl]oxy]hexahydro-1,2-dihydroxy-, [1S-(1 α ,2 α ,8 α ,8a α)]- (9CI) (CA INDEX NAME)

RN 164907-55-5 CAPLUS

3(2H)-Indolizinone, 8-[[(1,1-dimethylethyl)dimethylsilyl]oxy]hexahydro-1,2-CN dihydroxy-, $[1R-(1\alpha, 2\alpha, 8\beta, 8a\beta)]$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 106 OF 298 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

1995:510604 CAPLUS

DOCUMENT NUMBER:

123:33469

TITLE:

Stereocontrolled syntheses of polyhydroxy

indolizidines, including 8a-epi-, 6,8a-diepi- and 1,6-diepi-castanospermine, starting from malic acid

AUTHOR(S):

Leeper, Finian J.; Howard, Steven CORPORATE SOURCE:

SOURCE:

University Chemical Laboratory, Cambridge, CB2 1EW, UK

Tetrahedron Letters (1995), 36(13), 2335-8

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER:

DOCUMENT TYPE:

LANGUAGE:

OTHER SOURCE(S):

Elsevier

Journal English

CASREACT 123:33469

GΙ

Ι

Stereocontrolled total syntheses of one trihydroxyindolizidine and three tetrahydroxyindolizidines, e.g. I, all diastereoisomers of castanospermine, are described which use malic acid as the only chiral starting material.

Absolute stereochemistry.

RN 163811-97-0 CAPLUS CN 3(2H)-Indolizinone, 1-(benzoyloxy)-1,5,6,8a-tetrahydro-, (1R-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 163812-01-9 CAPLUS
CN 3(2H)-Indolizinone, 1-(benzoyloxy)hexahydro-7,8-dihydroxy-,
[1R-(1α,7α,8β,8aα)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 163812-02-0 CAPLUS CN 3(2H)-Indolizinone, 7,8-bis(acetyloxy)-1-(benzoyloxy)hexahydro-, $[1R-(1\alpha,7\alpha,8\beta,8a\alpha)]-$ (9CI) (CA INDEX NAME)

RN 163812-03-1 CAPLUS

CN 3(2H)-Indolizinone, 1-(benzoyloxy)hexahydro-7,8-bis[(methylsulfonyl)oxy]-, [1R-(1α ,7 α ,8 β ,8 α)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 163812-07-5 CAPLUS

CN 3(2H)-Indolizinone, 1-(benzoyloxy)hexahydro-8-hydroxy-7-(phenylseleno)-, [1R- $(1\alpha, 7\alpha, 8\beta, 8a\alpha)$]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 163812-08-6 CAPLUS

CN 3(2H)-Indolizinone, 1-(benzoyloxy)-1,5,8,8a-tetrahydro-8-hydroxy-, $[1R-(1\alpha,8\beta,8a\alpha)]-$ (9CI) (CA INDEX NAME)

RN 163812-10-0 CAPLUS

CN 3(2H)-Indolizinone, 6,7,8-tris(acetyloxy)-1-(benzoyloxy)hexahydro-, [1R-(1α ,6 β ,7 α ,8 β ,8 α)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 163812-12-2 CAPLUS

CN 3(2H)-Indolizinone, 1-(benzoyloxy)hexahydro-6,7,8-trihydroxy-, [1R-(1α , 6α , 7α , 8β , $8a\alpha$)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

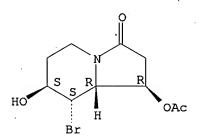
IT 163811-98-1P

RL: SPN (Synthetic preparation); PREP (Preparation) (stereocontrolled syntheses of polyhydroxy indolizidines, including epi- and diepicastanospermine starting from malic acid)

RN 163811-98-1 CAPLUS

CN 3(2H)-Indolizinone, 1-(acetyloxy)-8-bromohexahydro-7-hydroxy-, $[1R-(1\alpha,7\alpha,8\beta,8a\alpha)]$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 107 OF 298 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1995:425364 CAPLUS

DOCUMENT NUMBER: 123:56541

TITLE: Synthesis of 8-amino-3-oxoindolizidine-1-carboxylic acid derivatives as conformationally restricted

AUTHOR(S):

CORPORATE SOURCE:

templates for use in design of peptide mimetics Gomez Monterrey, Isabel Maria; Gonzalez-Muniz,

Rosario; Herranz, Rosario; Garcia-Lopez, Maria Teresa Instituto Quimica Medica, C.S.I.C., Madrid, 28006,

Spain

SOURCE:

Tetrahedron (1995), 51(9), 2729-36

CODEN: TETRAB; ISSN: 0040-4020

PUBLISHER:
DOCUMENT TYPE:
LANGUAGE:

Elsevier Journal English

OTHER SOURCE(S): CASREACT 123:56541

GI .

AB The synthesis of new 8-amino-3-oxoindolizidine-1-carboxylic acid esters I (Boc = Me3CO2C; R = Me, Et) with different stereochem. at positions 1, 8, and 8a is described. Three different paths from ornithine derivs. have been utilized. Compds. I can be employed as new templates in synthetic analogs of bioactive peptides.

TT 164223-14-7P 164223-15-8P 164323-61-9P 164323-62-0P 164323-63-1P 164323-64-2P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of amino(oxo)indolizidinecarboxylates as conformationally restricted dipeptide templates)

RN 164223-14-7 CAPLUS

CN 1-Indolizinecarboxylic acid, 8-[[(1,1-dimethylethoxy)carbonyl]amino]octahy dro-3-oxo-, methyl ester, [1S-(1 α ,8 β ,8a β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 164223-15-8 CAPLUS

CN 1-Indolizinecarboxylic acid, 8-[[(1,1-dimethylethoxy)carbonyl]amino]octahy dro-3-oxo-, ethyl ester, [1S-(1 α ,8 β ,8a β)]- (9CI) (CA INDEX NAME)

RN 164323-61-9 CAPLUS

CN 1-Indolizinecarboxylic acid, 8-[[(1,1-dimethylethoxy)carbonyl]amino]octahy dro-3-oxo-, methyl ester, [1R-(1 α ,8 α ,8a α)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 164323-62-0 CAPLUS

CN 1-Indolizinecarboxylic acid, 8-[[(1,1-dimethylethoxy)carbonyl]amino]octahy dro-3-oxo-, methyl ester, [1R-(1 α ,8 α ,8a β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 164323-63-1 CAPLUS

CN 1-Indolizinecarboxylic acid, 8-[[(1,1-dimethylethoxy)carbonyl]amino]octahy dro-3-oxo-, ethyl ester, [1R-(1 α ,8 α ,8a α)]- (9CI) (CA INDEX NAME)

RN 164323-64-2 CAPLUS

CN 1-Indolizinecarboxylic acid, 8-[[(1,1-dimethylethoxy)carbonyl]amino]octahy dro-3-oxo-, ethyl ester, $[1R-(1\alpha,8\alpha,8a\beta)]-(9CI)$ INDEX NAME)

Absolute stereochemistry.

ANSWER 108 OF 298 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

1995:401217 CAPLUS

DOCUMENT NUMBER:

122:187625

TITLE:

[(alkoxyphenyl)pyrrolyl]indolizines and

[(alkoxyphenyl)pyrrolyl]quinolizines as antipsychotic

agents

INVENTOR(S):

Hadley, Michael Stewart; Johnson, Christopher Norbert;

Stemp, Geoffrey

PATENT ASSIGNEE(S):

Smithkline Beecham PLC, UK

SOURCE:

PCT Int. Appl., 21 pp. CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PA	TENT NO.		KIND DATE		APPLICATION NO.	DATE		
WC	9424129		A1	19941027	WO 1994-EP992	19940329 <		
	W: JP, US RW: AT, BI 0 693068 0 693068				GB, GR, IE, IT, LU, MC, EP 1994-912552	NL, PT, SE 19940329 <		
	R: BE, CI	H, DE,	FR, G	3, IT, LI,				
	08508509 5688790		T A	19960910 19971118		19940329 <		

PRIORITY APPLN. INFO.:

GB 1993-7400 WO 1994-EP992 A 19930408 W 19940329

OTHER SOURCE(S):

MARPAT 122:187625

GI

$$R^3$$
 R^5
 R^5
 R^5
 R^5
 R^5
 R^5
 R^5
 R^5

The title compds., 3-[2-(2-alkoxyphenyl)-1H-pyrrol-5-yl]indolzines and 4-[2-(2-alkoxyphenyl)-1H-pyrrol-5-yl]quinolizines I (R1 = alkyl; R2-R5 = H, alkyl, alkoxy, etc.; Y = 1-azabicyclo[4.3.0]nonyl, 1-azabicyclo[4.4.0]decyl, etc.) were disclosed as antipsychotic agents.an. Example compound, 3-[2-(3,5-dibromo-2-methoxyphenyl)-1H-pyrrol-5-yl]quinolizine (II) was prepared (mixts. of diastereomers).

IT 2740-00-3, 3(2H)-Indolizinone, hexahydro-, (+)-

II

RN 2740-00-3 CAPLUS

CN 3(2H)-Indolizinone, hexahydro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

L5 ANSWER 109 OF 298 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

1995:333384 CAPLUS

DOCUMENT NUMBER:

122:187834

TITLE:

Aza-[2,3]-Wittig rearrangements of vinylaziridines as

a novel entry to indolizidine alkaloids.

Enantioselective total synthesis of indolizidine 209D

AUTHOR(S):

Ahman, Jens; Somfai, Peter

CORPORATE SOURCE:

Univ. Lund, Chem. Cent. Lund Inst. Technol., Lund,

S-221 00, Swed.

SOURCE:

Tetrahedron Letters (1995), 36(2), 303-6

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: DOCUMENT TYPE:

Elsevier Journal

LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 122:187834

GI

Me[CH₂]₅

H

I Me
$$\left\{ \text{CH}_{2} \right\}_{5}$$

NCH₂CO₂CMe₃

II

AB An enantioselective total synthesis of indolizidine 209D (I) from 2,3-epoxy-1-hexanol is described. The key step in the sequence involves an aza-[2,3]-Wittig rearrangement of vinylaziridine II to yield tert-Bu cis-6-hexyl-1,2,3,6-tetrahydropyridine-2-carboxylate in 98% yield and as a single detectable diastereomer.

IT 161404-23-5P

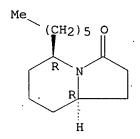
> RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(aza-[2,3]-Wittig rearrangement of vinylaziridine in total synthesis of indolizidine 209D)

RN 161404-23-5 CAPLUS

3(2H)-Indolizinone, 5-hexylhexahydro-, (5R-trans)- (9CI) (CA INDEX NAME) CN

Absolute stereochemistry.



L5 ANSWER 110 OF 298 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

1995:237440 CAPLUS

DOCUMENT NUMBER:

122:133484

TITLE:

Stereoselective synthesis of (+) - and

(-)-lentiginosine

AUTHOR(S):

Gurjar, M. K.; Ghosh, Lakshmi; Syamala, M.; Jayasree,

CORPORATE SOURCE:

Indian Institute of Chemical Technology, Hyderabad,

500 007, India

SOURCE: -

Tetrahedron Letters (1994), 35(47), 8871-2

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER:

Elsevier

DOCUMENT TYPE:

Journal English

LANGUAGE: OTHER SOURCE(S):

CASREACT 122:133484

GI

AB Simple routes to (1R,2R,8aR)- (I) and (1S,2S,8aS)-lentiginosine have been described, based on Sharpless asym. dihydroxylation, starting from (R)-and (S)-pipecolinic acids.

IT 160096-52-6P 160169-49-3P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (stereoselective synthesis of and lentiginosine)

RN 160096-52-6 CAPLUS

I

CN 3(2H)-Indolizinone, 1,2-bis(acetyloxy)hexahydro-, [1R- $(1\alpha, 2\beta, 8a\alpha)$]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 160169-49-3 CAPLUS

CN 3(2H)-Indolizinone, hexahydro-1,2-dihydroxy-, (1R,2S,8aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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CA SUBSCRIBER PRICE

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FULL ESTIMATED COST

SINCE FILE TOTAL

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FILE 'REGISTRY' ENTERED AT 06:36:44 ON 26 JUL 2007

L1 STRUCTURE UPLOADED

L2 44 S L1

L3 962 S L1 FULL

FILE 'CAPLUS' ENTERED AT 06:37:39 ON 26 JUL 2007

L4 357 S L3 FULL

L5 298 S L4 AND PY<2003

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FULL ESTIMATED COST 0.18 238.23

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ENTRY SESSION

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